

Nonadiabatic effects in the 4f 1-5d 1 absorption spectrum of a LiYF₄:Ce³⁺ crystal

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Abstract

We have modeled the 4f 1-5d 1 absorption spectrum of a LiYF₄:Ce³⁺ crystal at zero temperature using a microscopic model of the electron-phonon interaction and the real spectrum of LiYF₄ lattice vibrations. Effects caused by mixing of the wave functions of different states of the 5d 1 excited configuration of the Ce³⁺ ion, which is induced by the electron-phonon interaction, are considered based on the calculations of the second-, third-, and fourth-order exact moments of curvature of the spectrum envelope. We have shown that the large value of the splitting between the maxima of the bands in the absorption spectrum that correspond to transitions to the third and fourth 5d 1 levels is a result of the nonadiabatic interaction of 5d electrons with lattice vibrations. © 2014 Pleiades Publishing, Ltd.

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